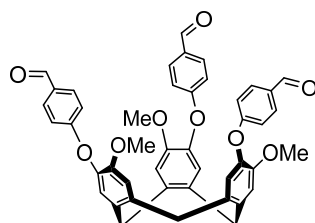
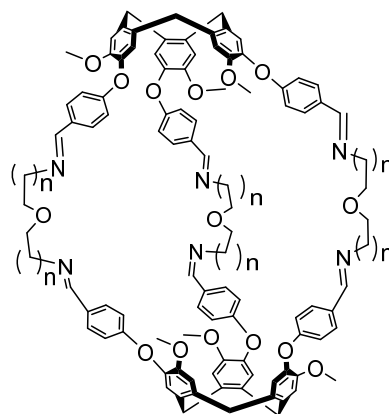


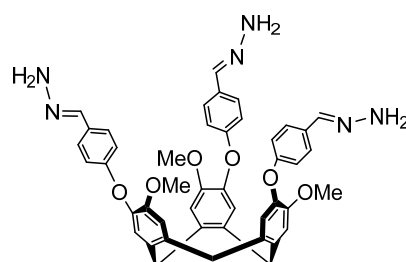
Compound Diagrams and meta-data



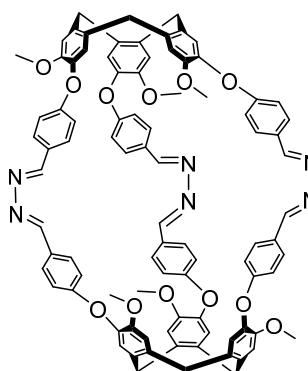
cavitand 1



$n = 1$ cryptophane (or crypto) 2
 $n = 2$ cryptophane 3



cavitand 4



Cryptophane (or crypto) 5

Folder “NMR” Nuclear Magnetic Resonance data

“Raw” – as collected data in FID or other format

“Spectra” – worked up spectra

Folder “XRay” Single Crystal X-ray Data

All structures:

name.cif (crystallographic information file with embedded calculated and observed structure factors and SHELX instruction file)

name.hkl (data file)

name.res (final SHELX results file)

Folder “HRMS and IR”

HRMS – high resolution mass spectra

IR – infrared spectra